

# New developments in the McStas neutron instrument simulation package

**Willendrup, Peter Kjær; Bergbäck Knudsen, Erik; Klinkby, Esben Bryndt; R. Nielsen, Torben; Farhi, E.; Filges, U.; Lefmann, K.**

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# New developments in the McStas neutron instrument simulation package

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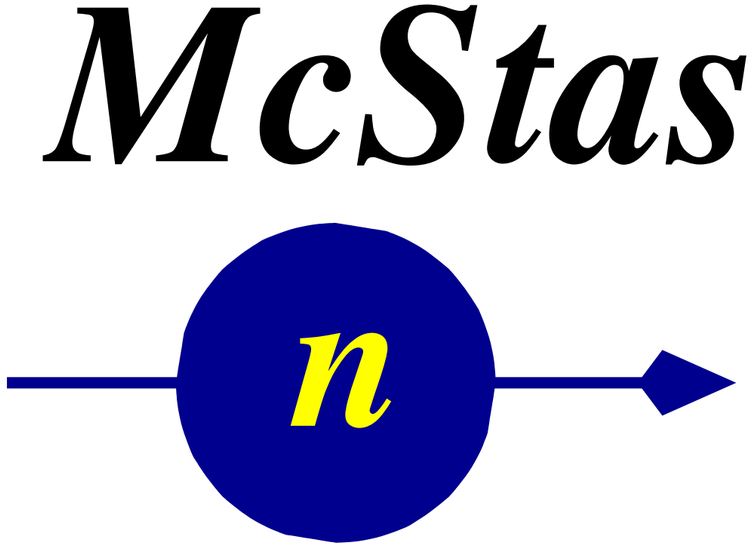
[4]ESS Neutronics Group, Sweden

[5]CS-group, Institut Laue-Langevin (ILL), France

[6]LDM, Paul Scherrer Institute (PSI), Switzerland

[7]eScience and Nano-Science centers, Niels Bohr Institute (NBI), Denmark





# Agenda

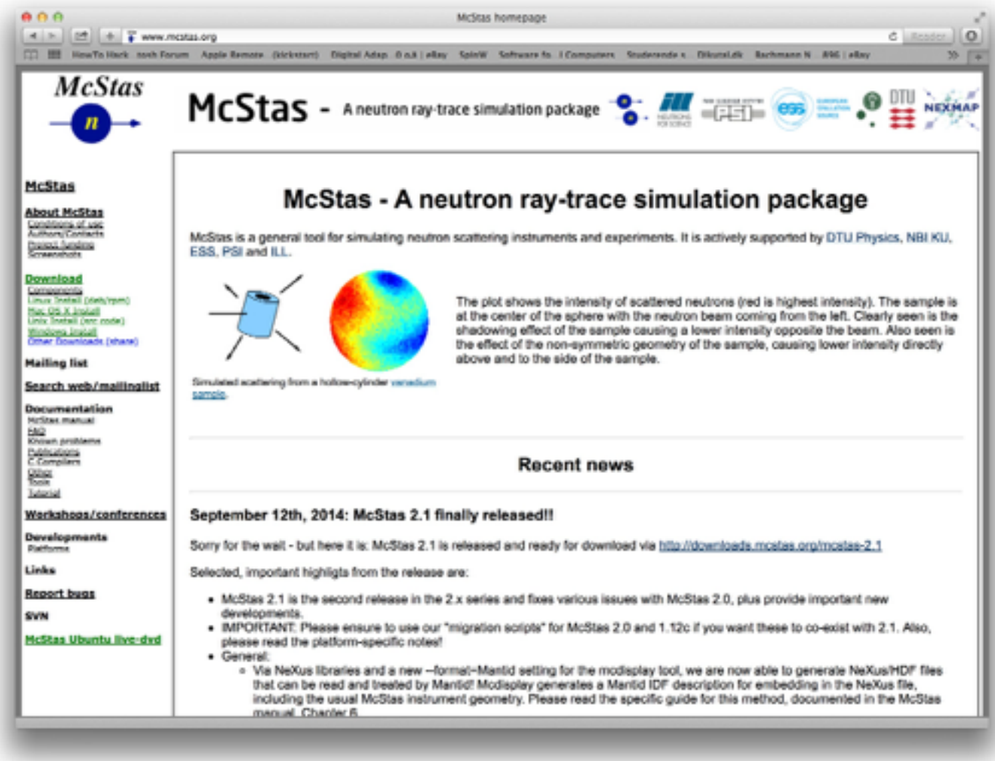
- A brief introduction to McStas, Monte Carlo & raytracing

- Highlighted new features in McStas 2.1
  - McStas-MCNP for background estimates
  - McStas-Mantid event processing
  - Speedup in Single_crystal.comp

# McStas Introduction

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at DTU Physics, ILL, PSI, Uni CPH, **ESS**
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
- Currently 2.5+1 people full time plus students

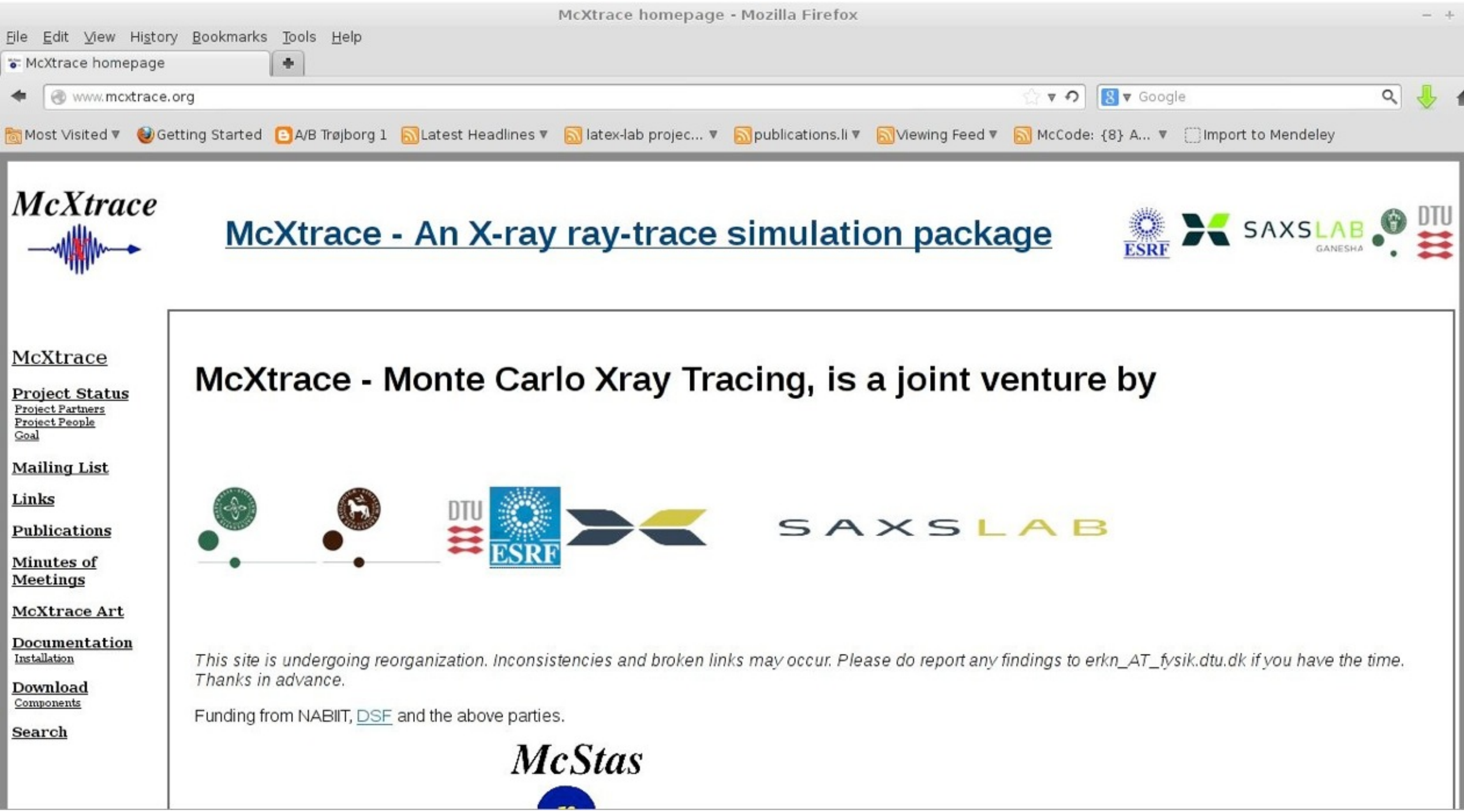
GNU GPL license
Open Source




Project website at
http://www.mcstas.org

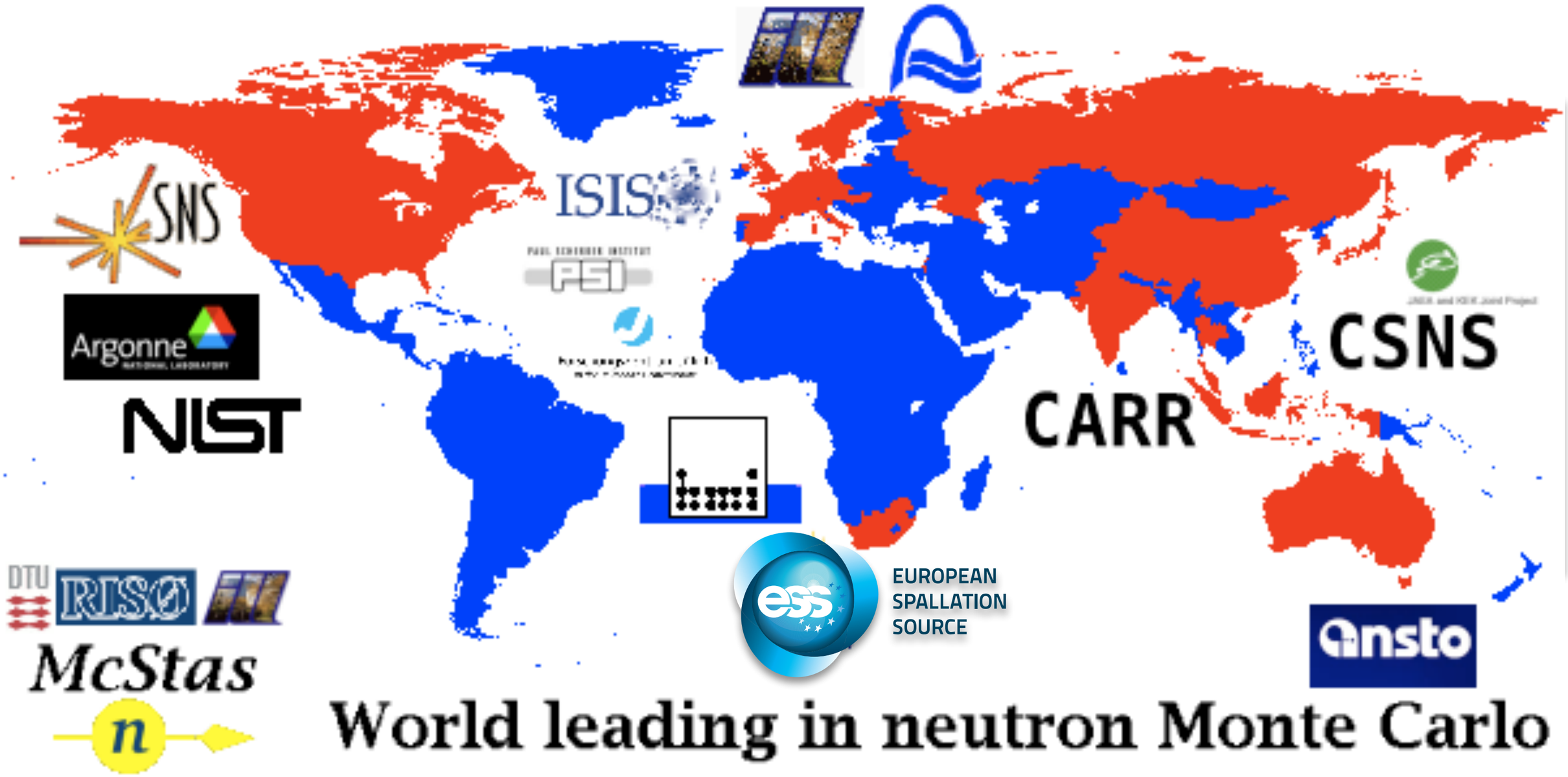
mcstas-users@mcstas.org mailinglist

**New developments in McStas**



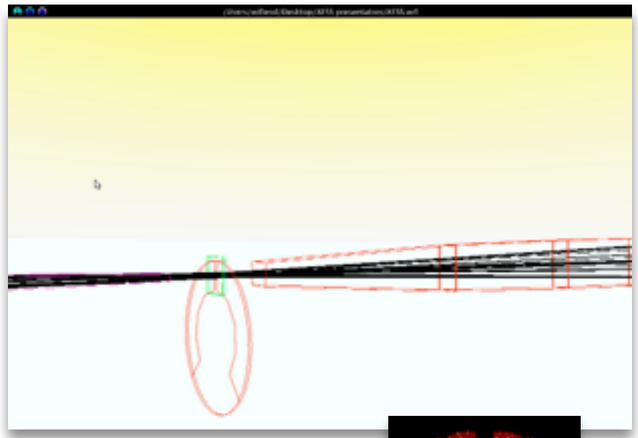

**New developments in McStas**

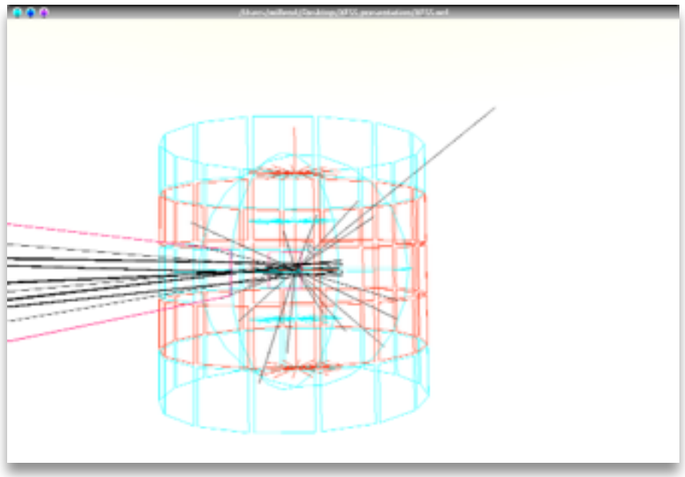
# McStas Introduction

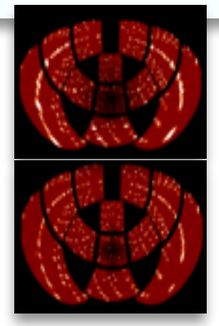


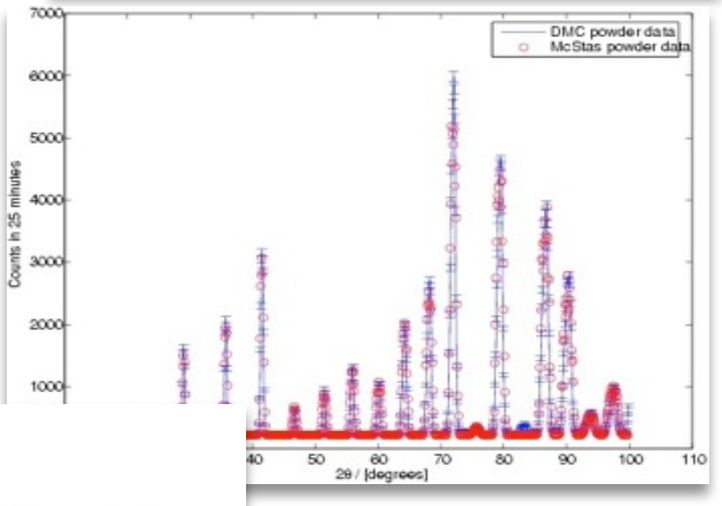

New developments in McStas

# What is McStas used for?



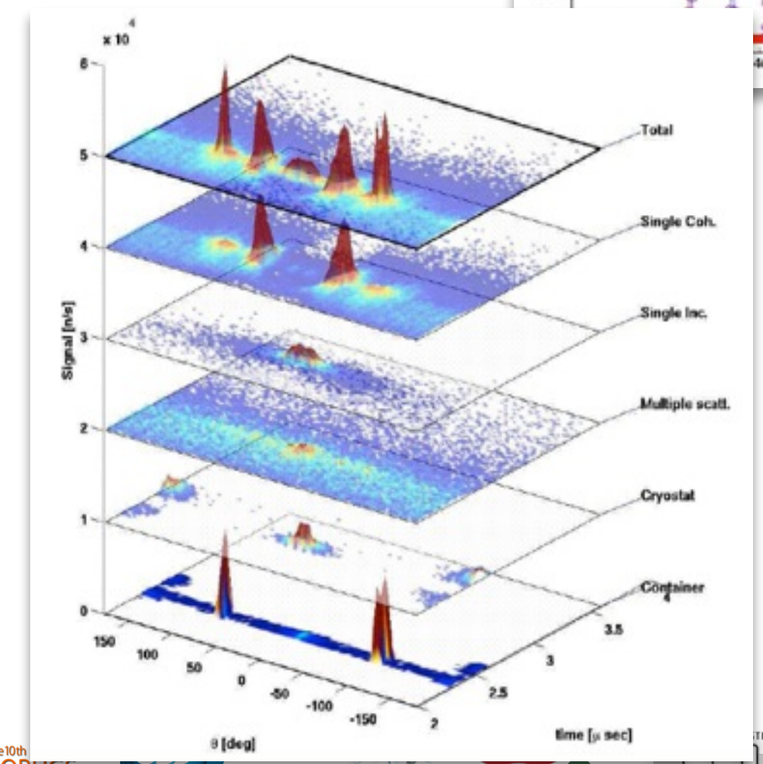


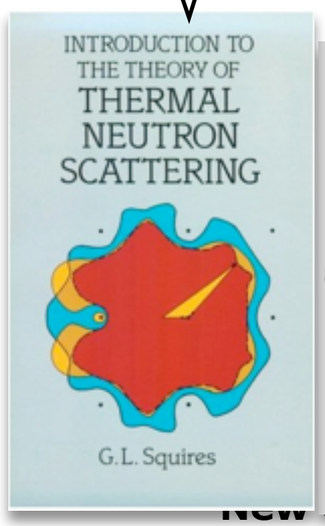


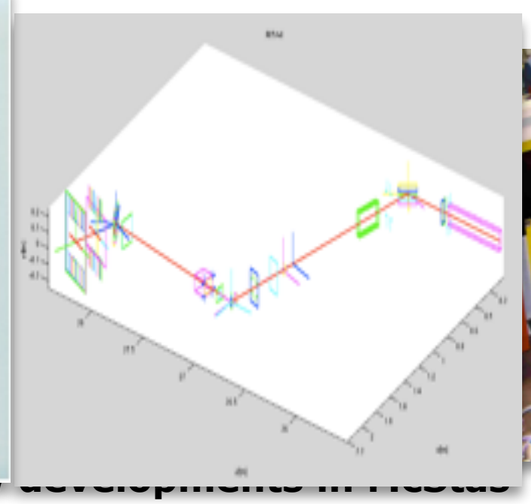



- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

(KU, DTU)

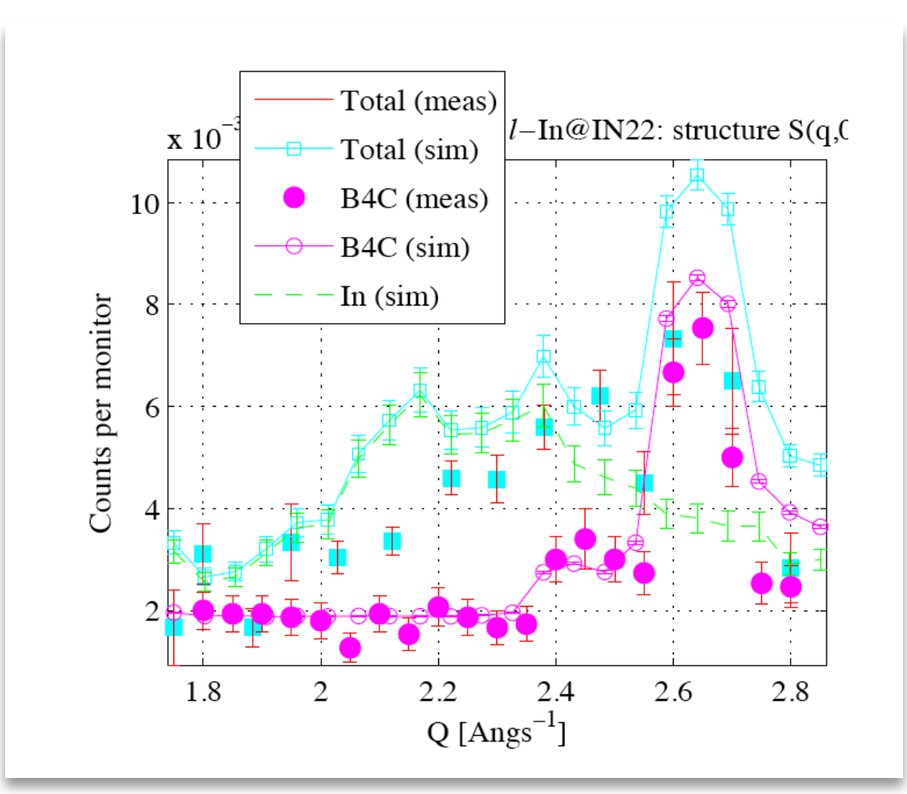


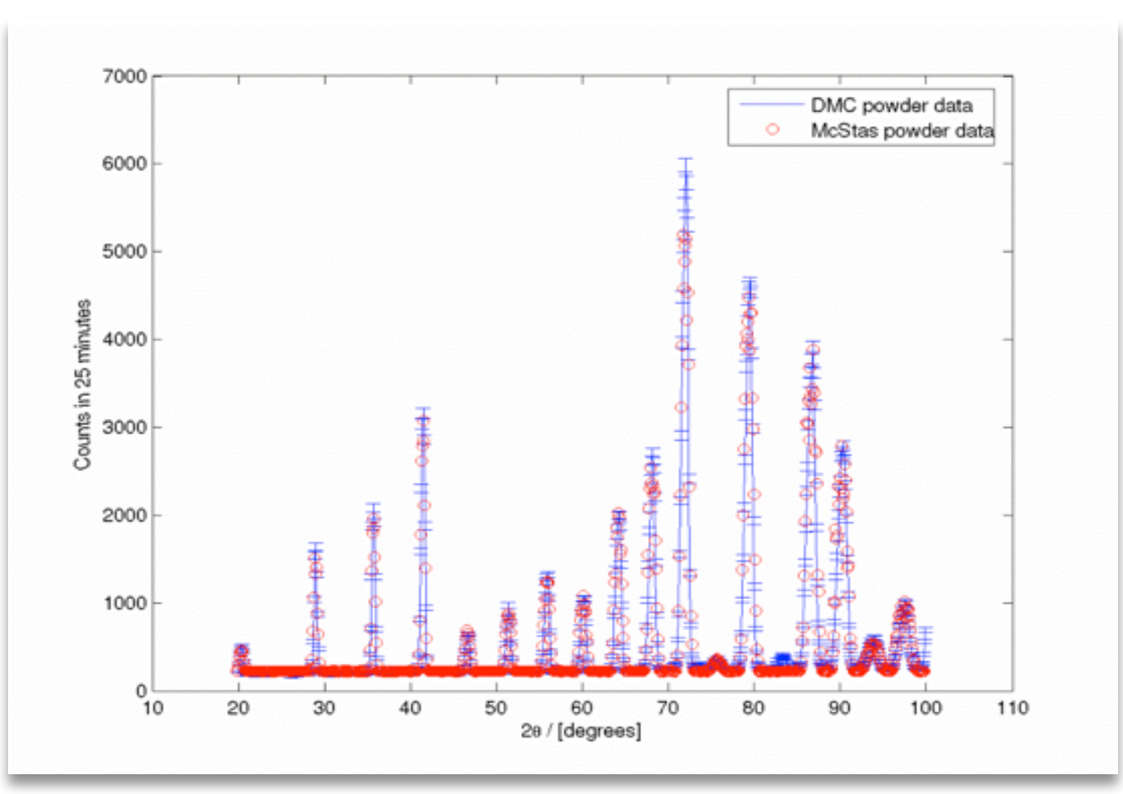



# Reliability - cross comparisons

- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agrees very well with other packages (NISP, Vitess, IDEAS, RESTRAX, ...)
- Experimental line shapes are within 5%
- Absolute intensities are within 10%
- Common understanding: McStas and similar codes are reliable




E. Farhi, P. Willendrup et al., in preparation




P. Willendrup et al., Physica B, 386, (2006), 1032.

**New developments in McStas**

Neutron ray/package:

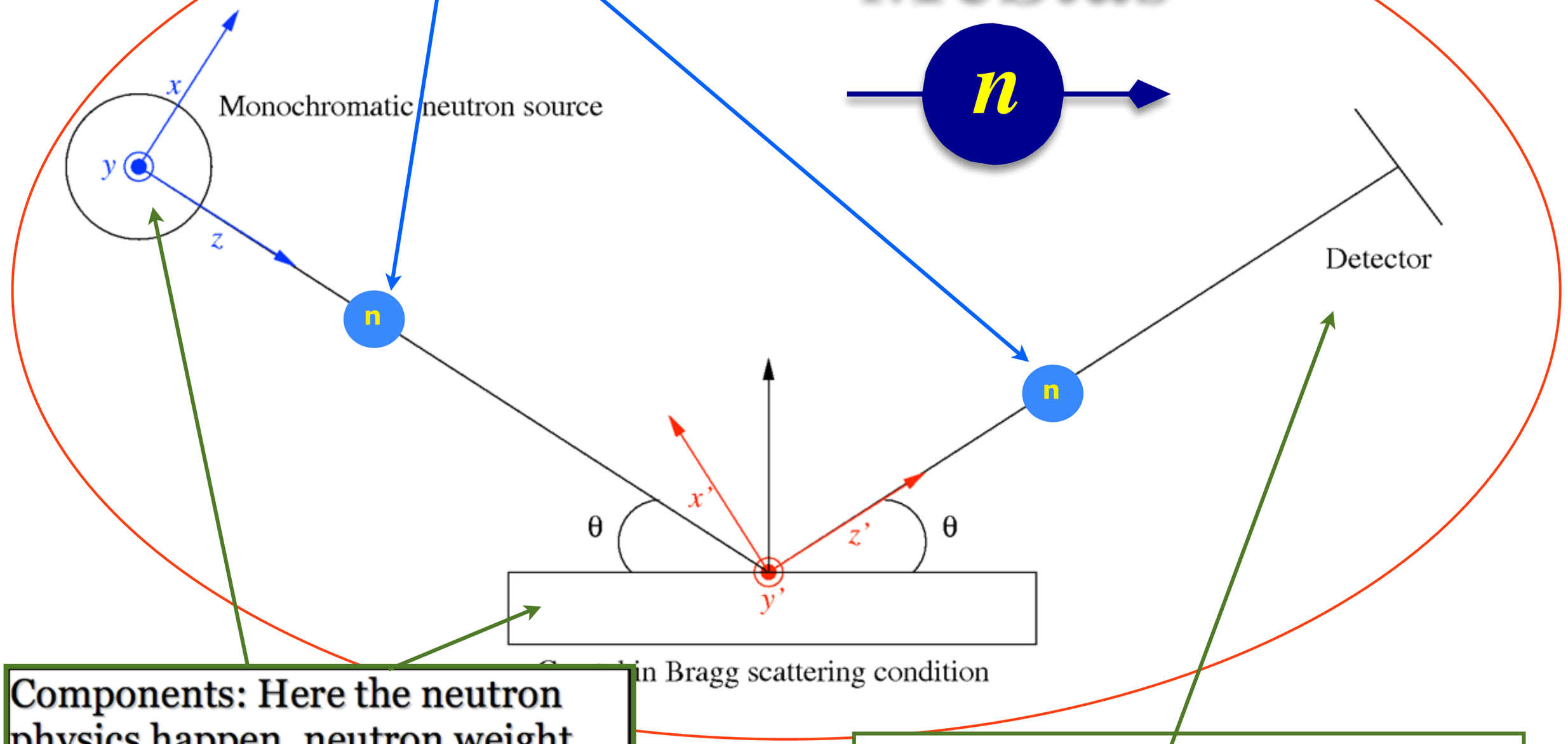
Weight (p): # neutrons (left) in the package
Coordinates (x,y,z)
Velocity ($v_x$,$v_y$,$v_z$)
Spin ($s_x$,$s_y$,$s_z$)

Time (t)

Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.

# *McStas*



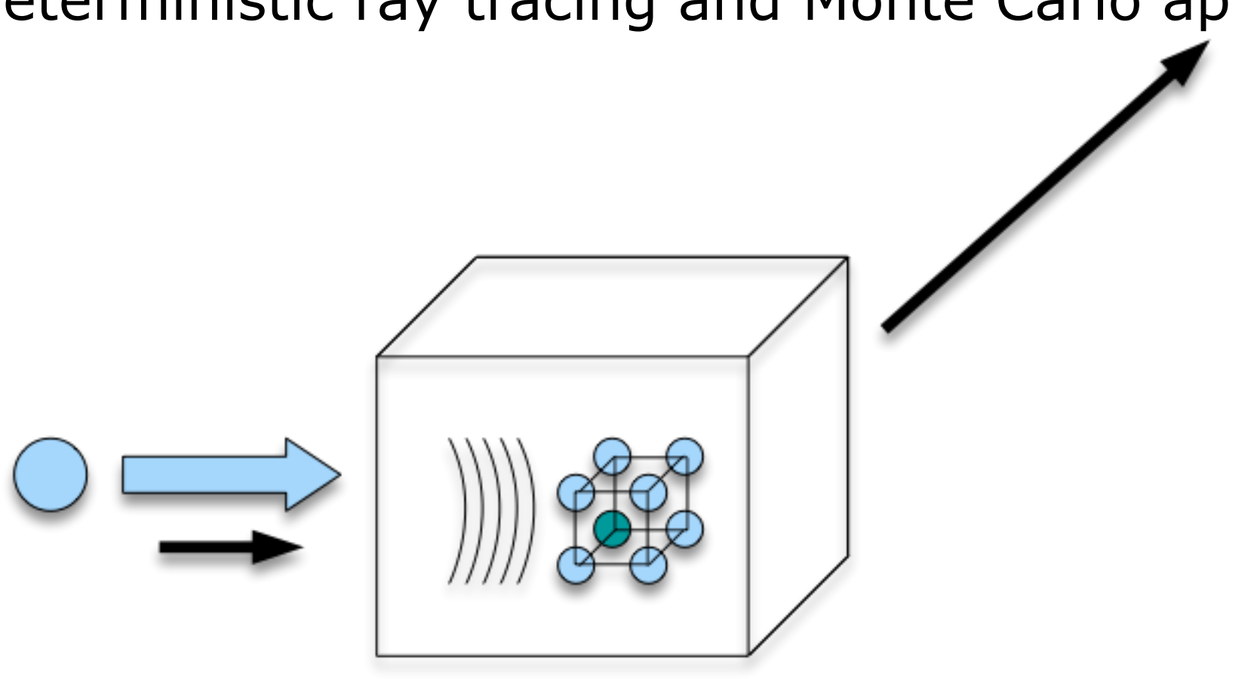




Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.

Local, internal coordinate system!

# Elements of Monte-Carlo raytracing

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- Uses Monte Carlo sampling of "complicated" distributions and stochastic processes and multiple outcomes with known probabilities are involved
- - I.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach



- Result: A realistic and efficient transport of neutrons in the thermal and cold range

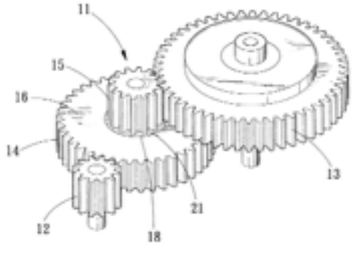
# McStas overview

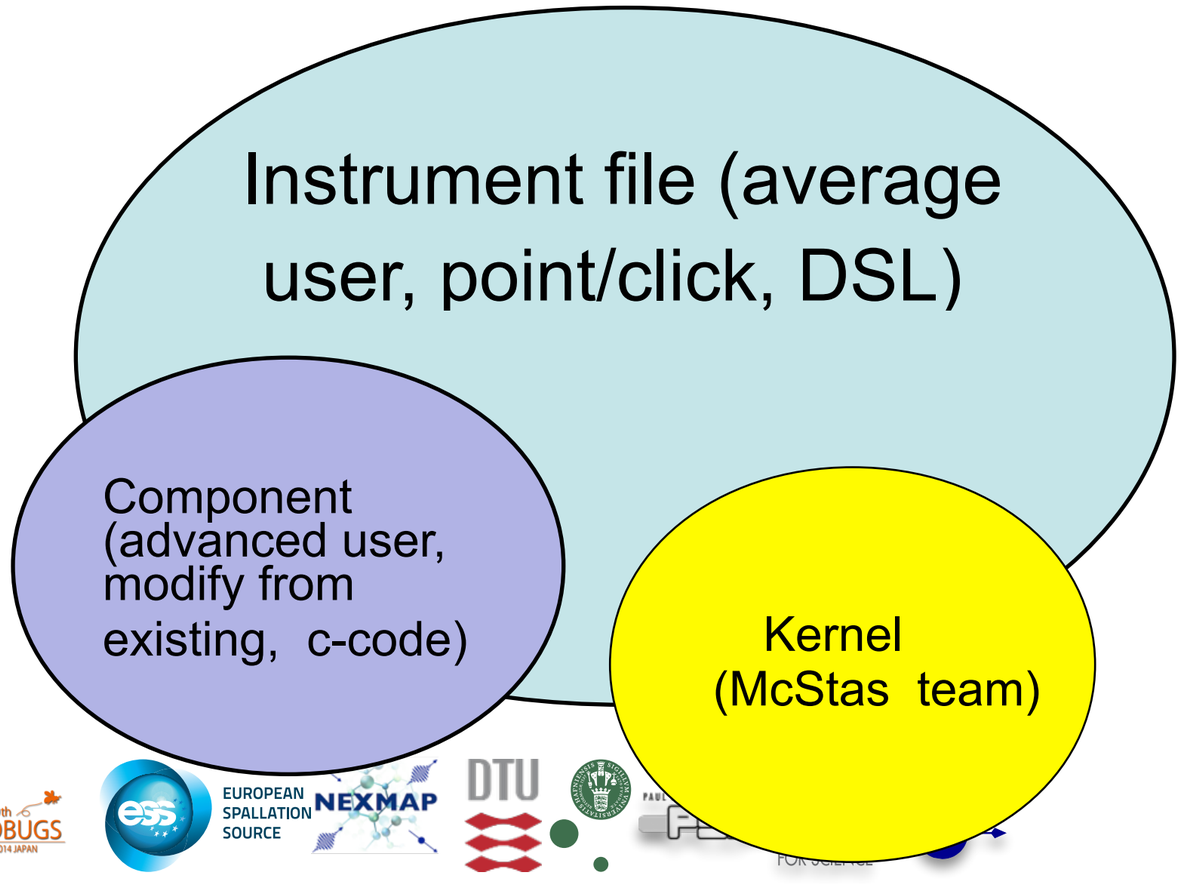
- Portable code (Unix/Linux/Mac/Windoze)

- Ran on everything from iPhone to 1000+ node cluster!

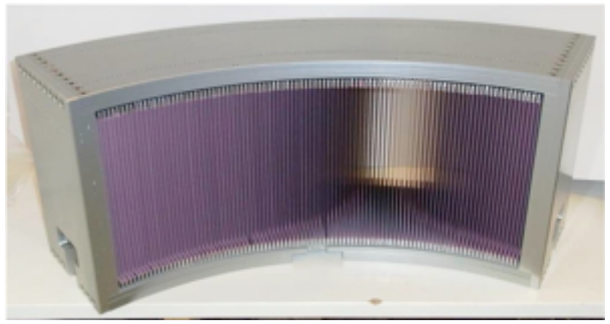
- 'Component' files (~150) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps

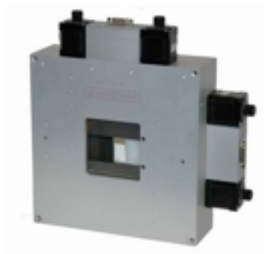
- DSL + ISO-C code gen.

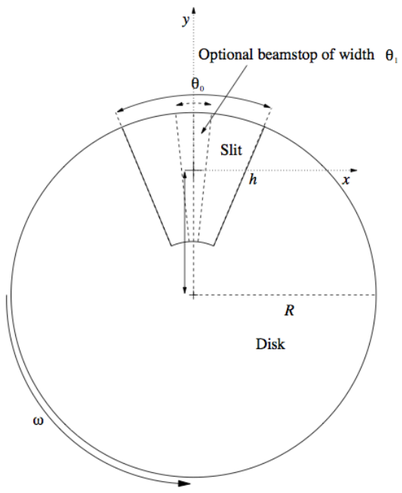


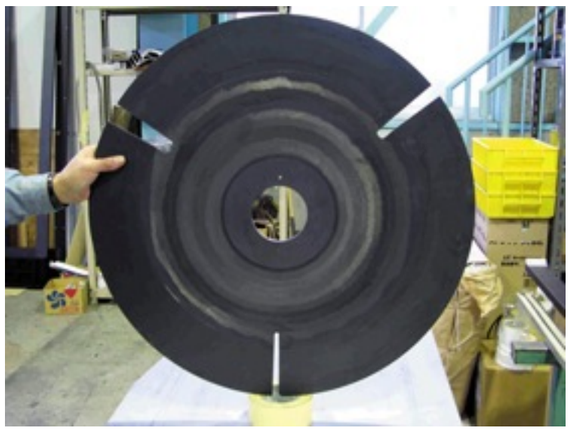



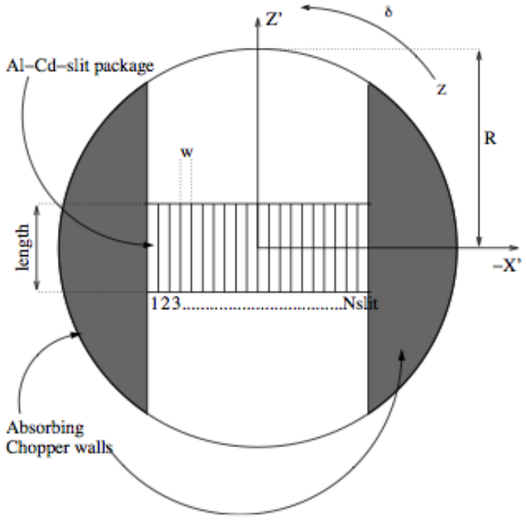
# Neutron optics and other instrument components

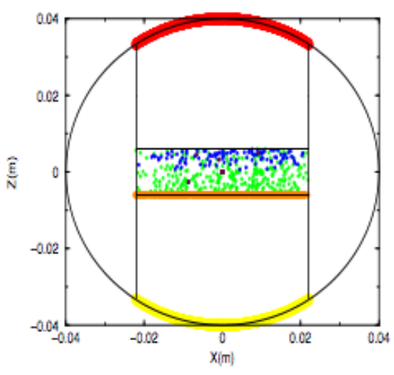


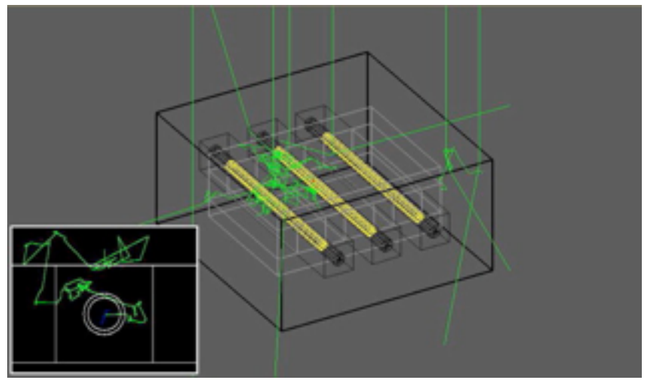






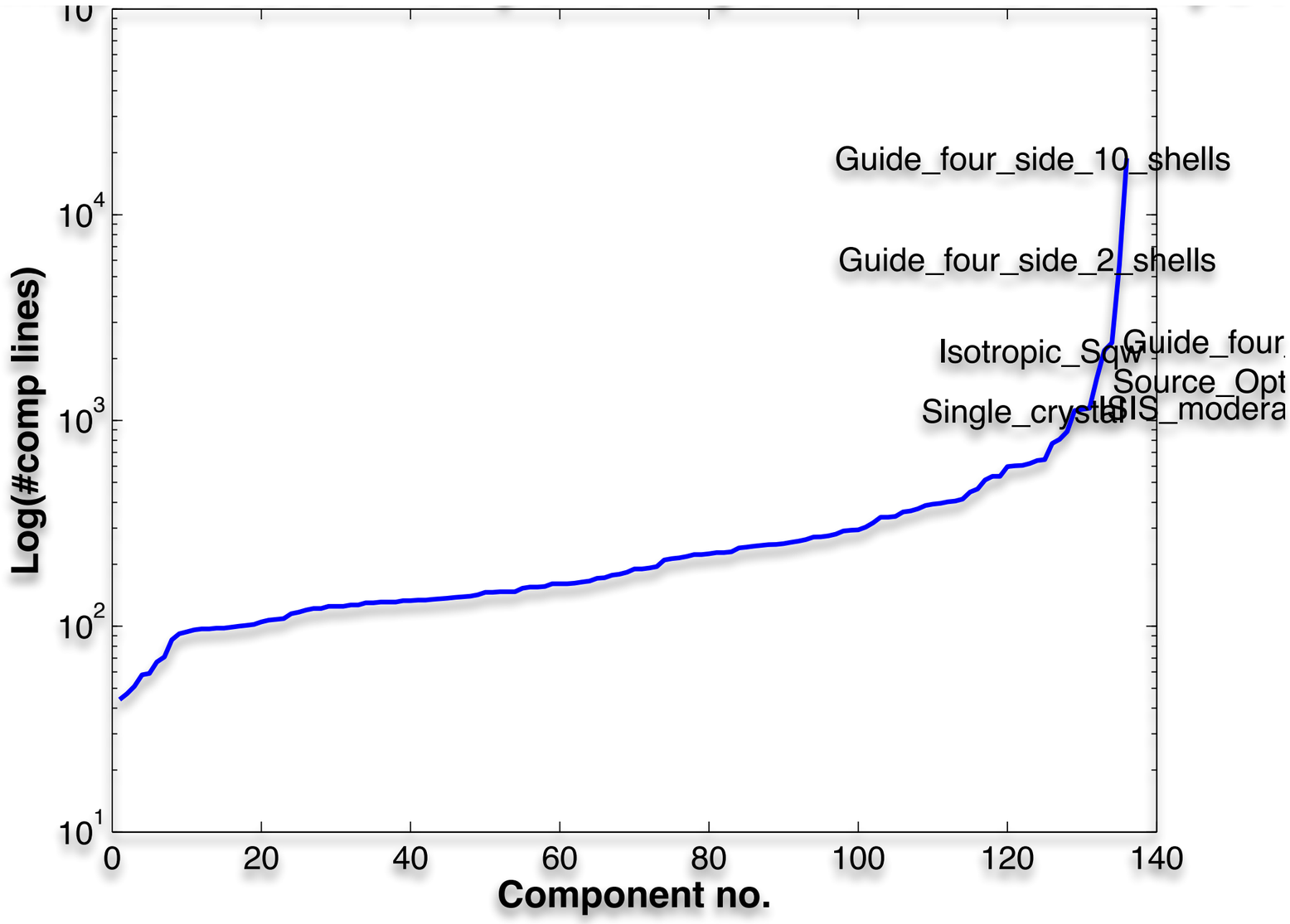



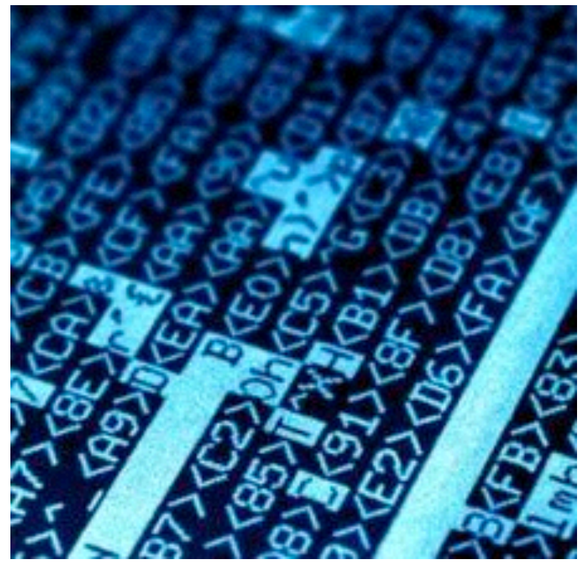
## New developments in McStas

# Writing new comps or understanding existing is not that complex...

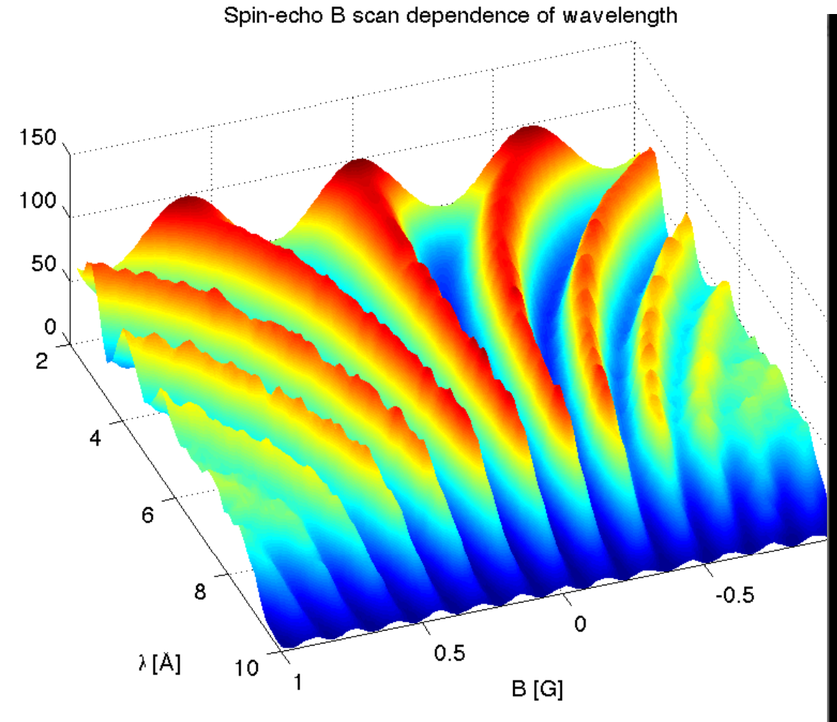
- Check our long list of components and look inside... Most of them are quite simple and short... Statistics:

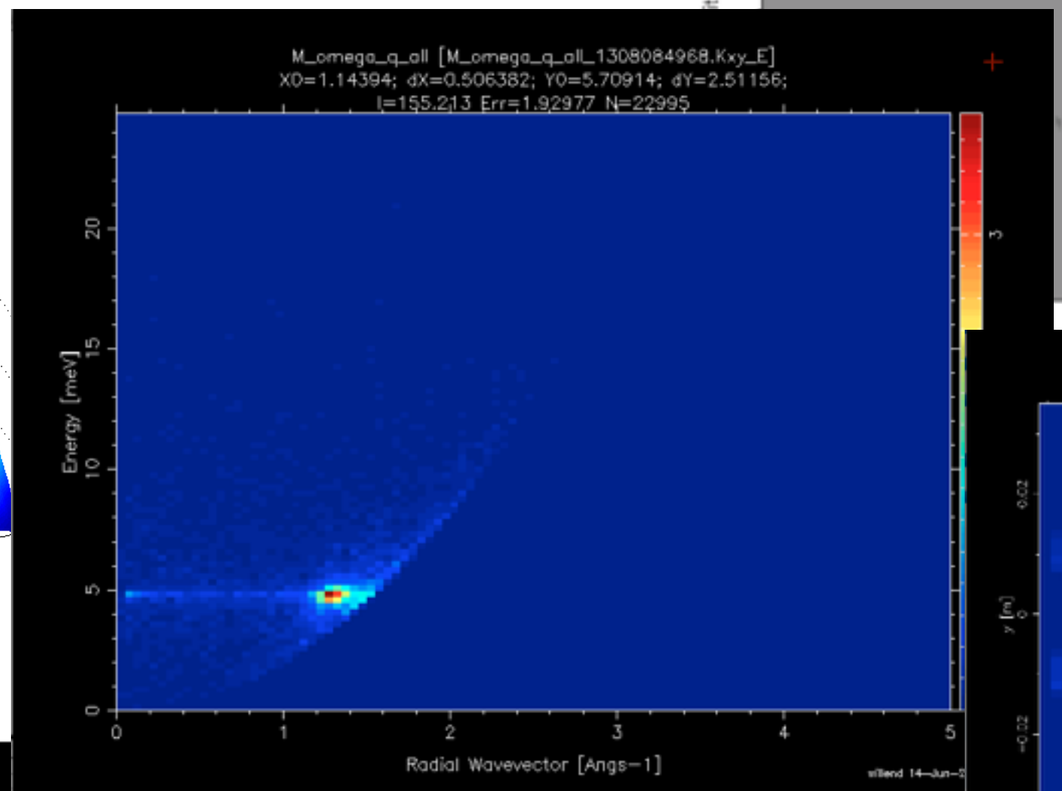
**Number of lines of code per component - 165 comps in total**

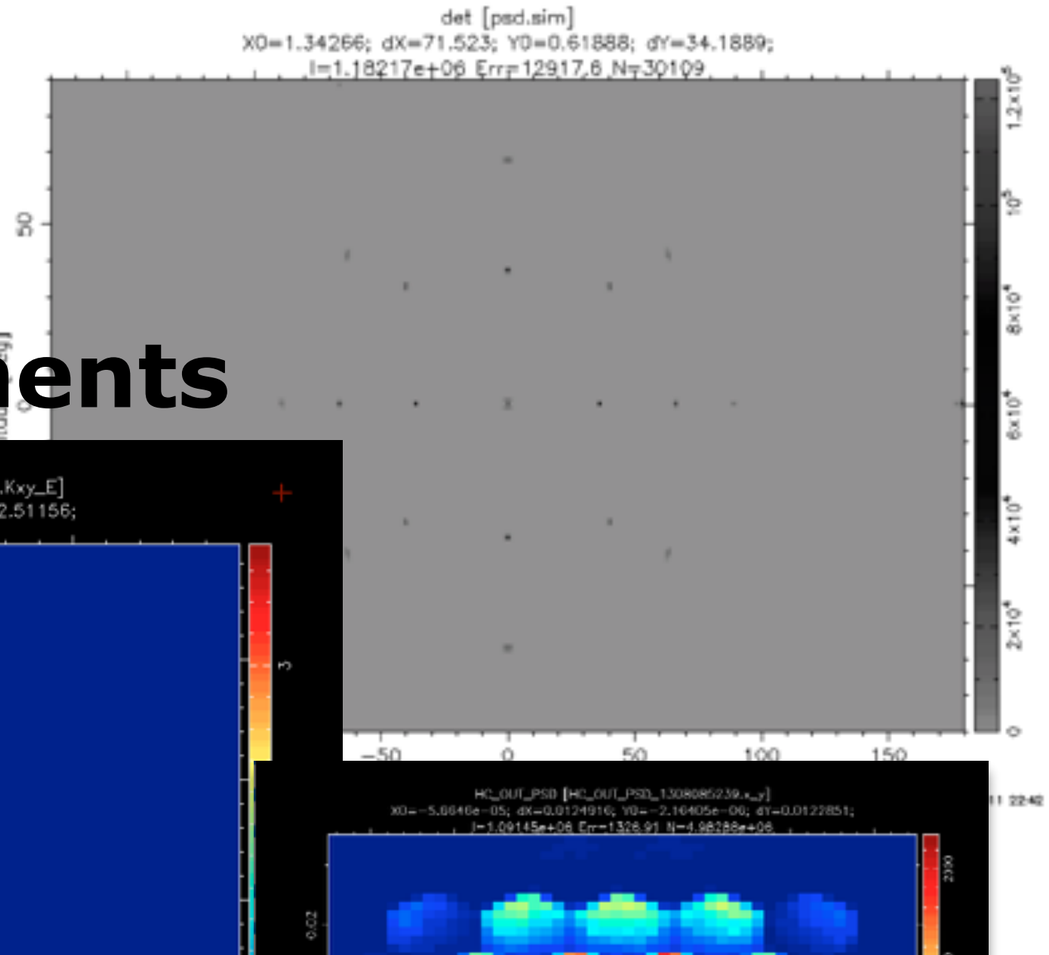


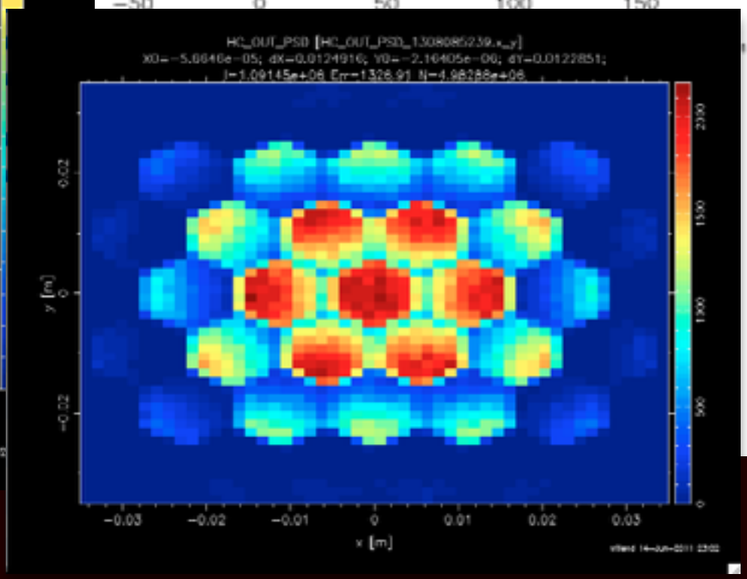



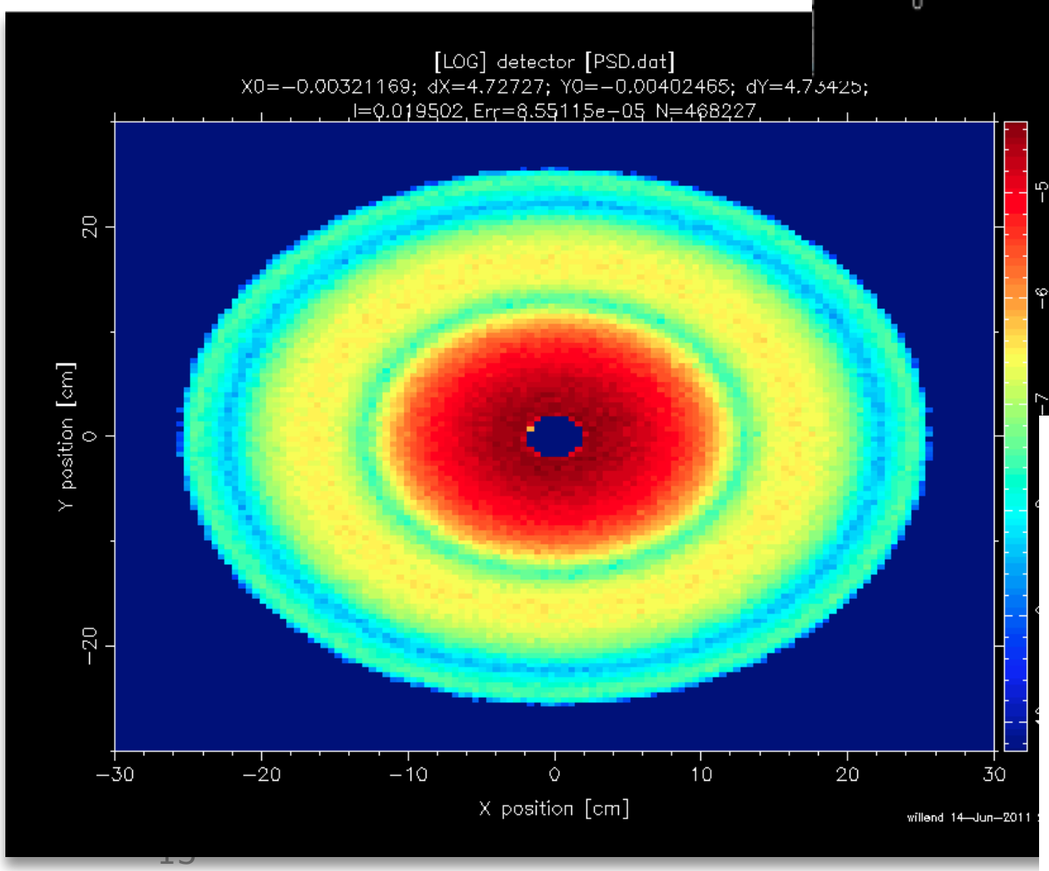
# Example suite: 123 instruments

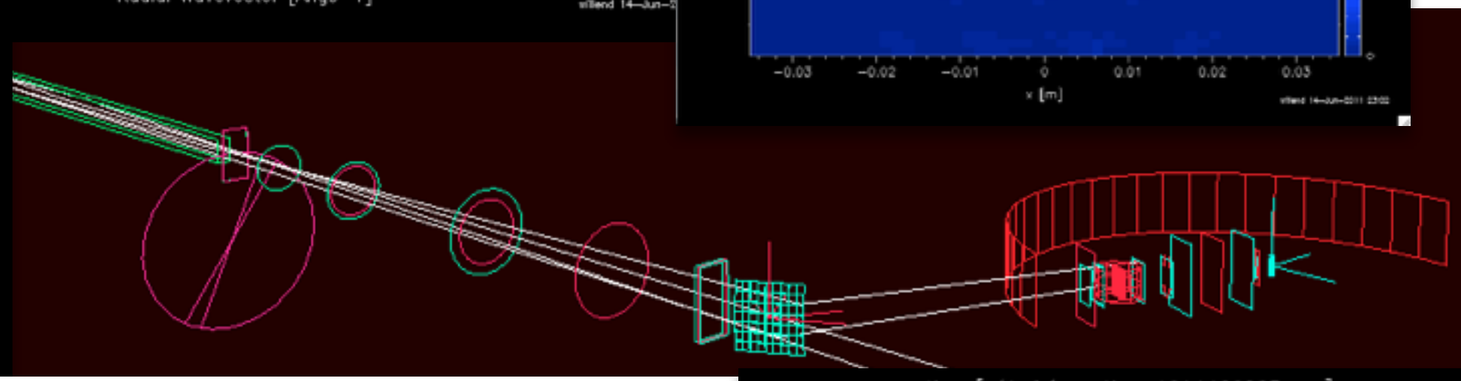


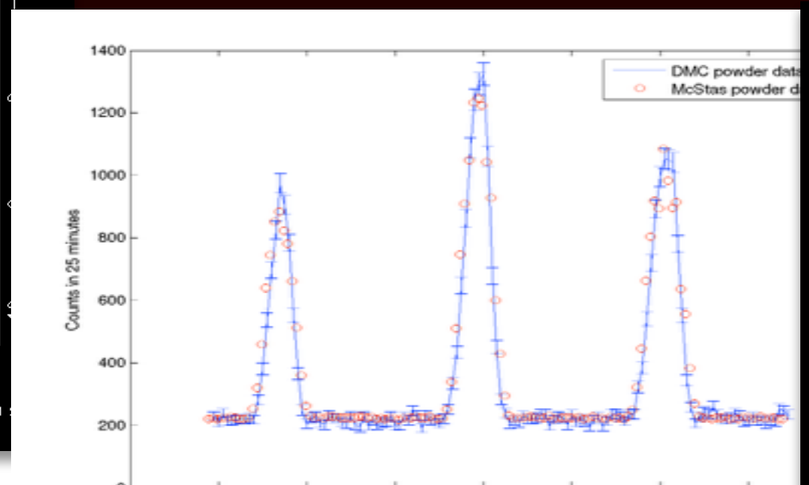



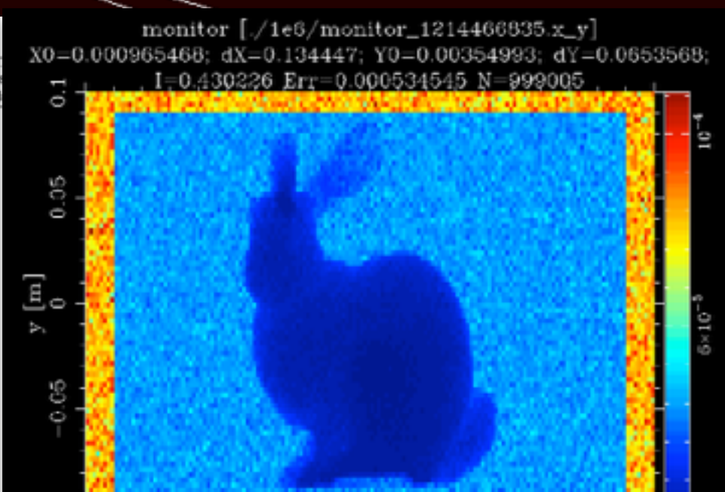



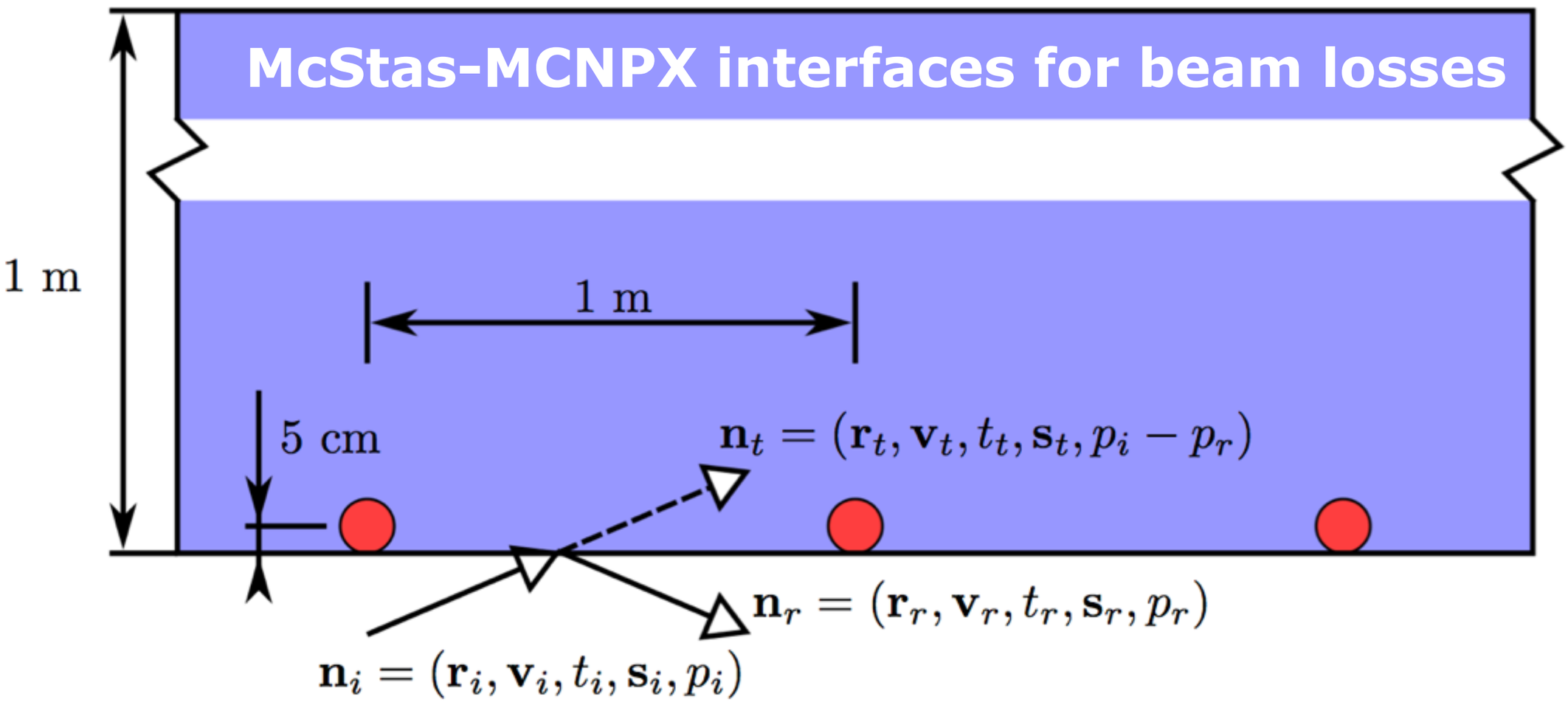





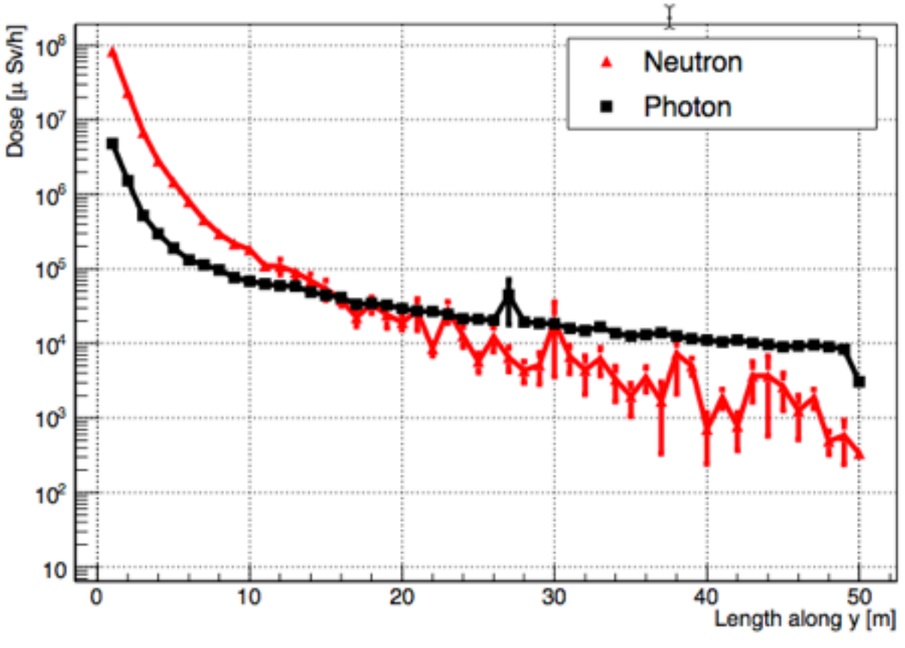
# McStas-MCNPX interfaces for beam losses

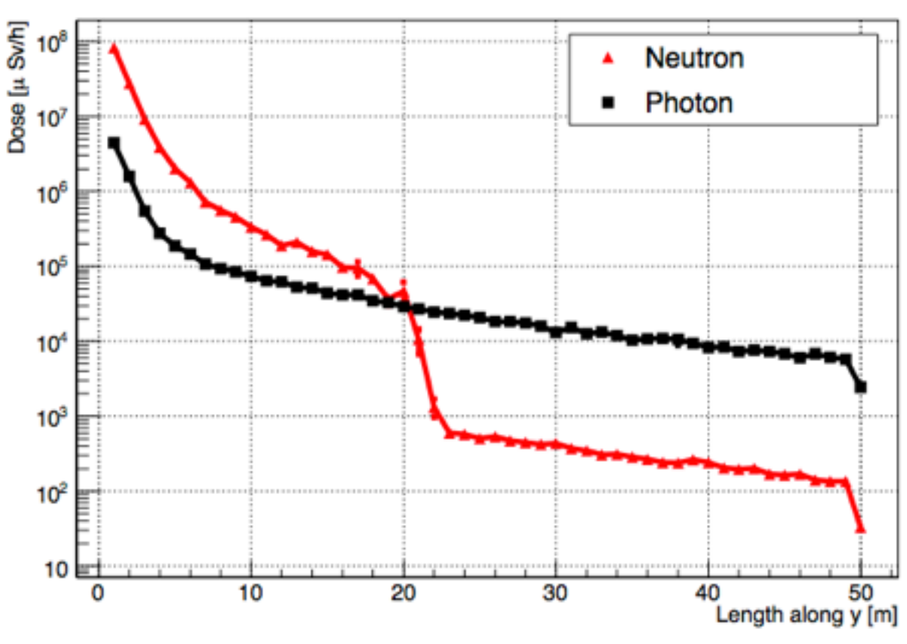



MCNPX

SSR SSW

McStas

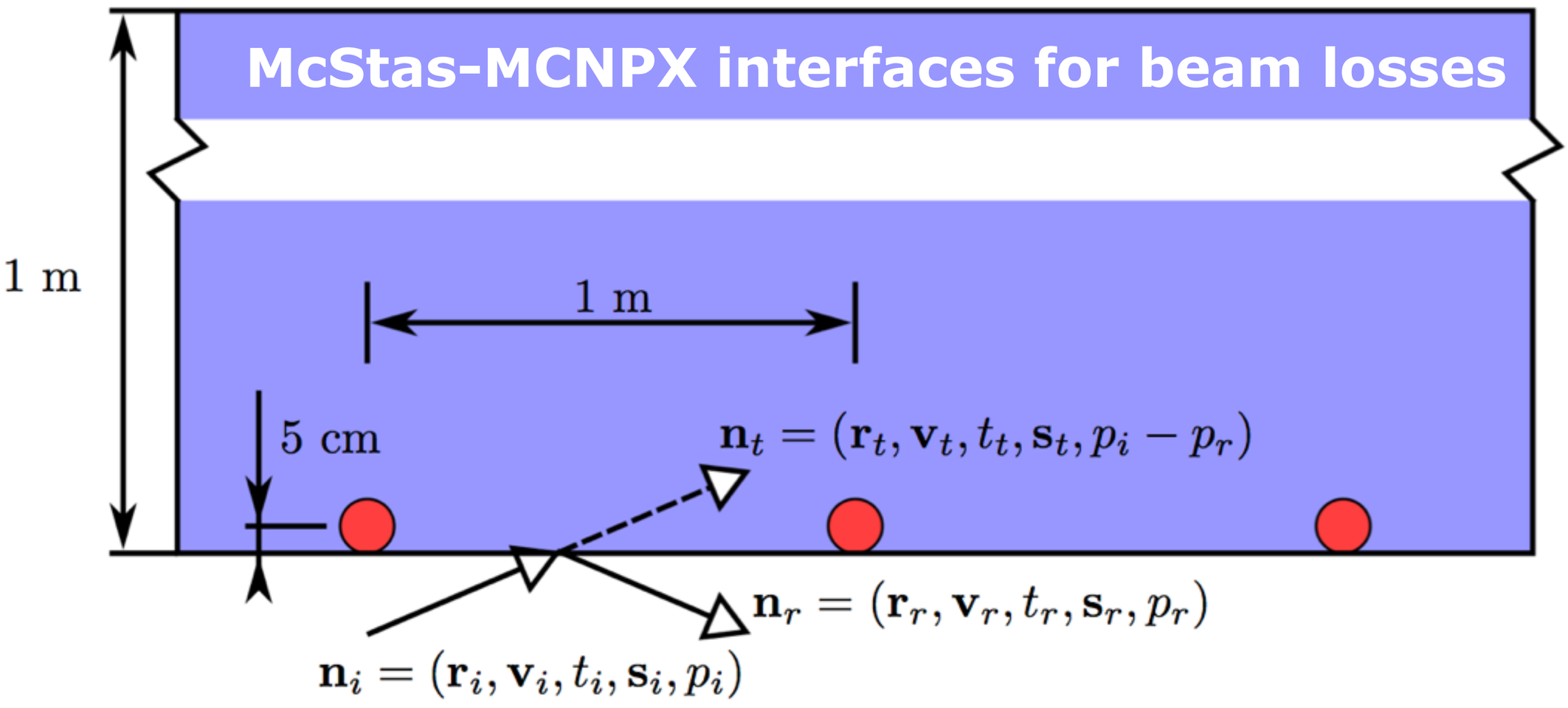



Collaboration
DTU Nutech
DTU Fysik
ESS

PSI NEUTRONS FOR SCIENCE McStas

# McStas-MCNPX interfaces for beam losses

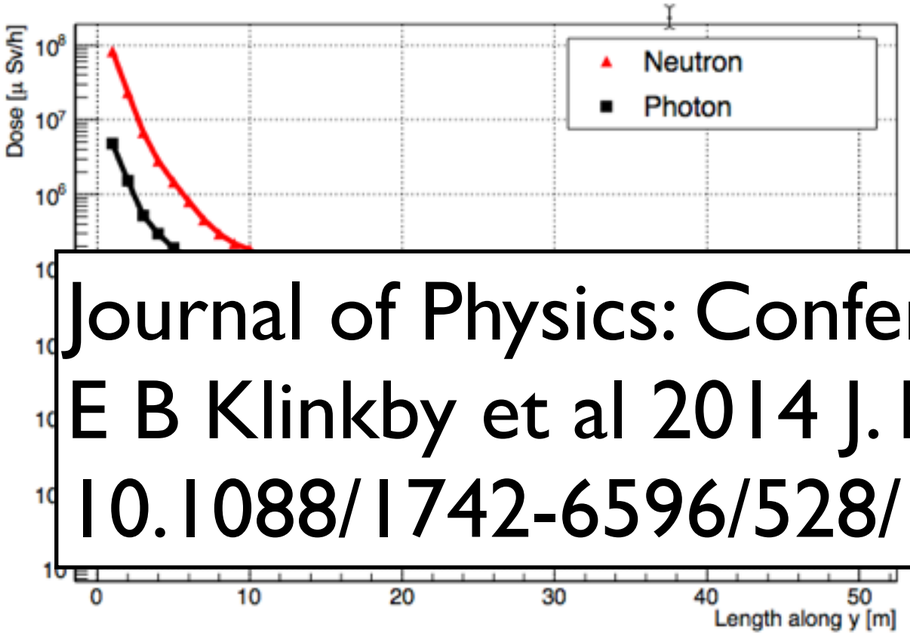


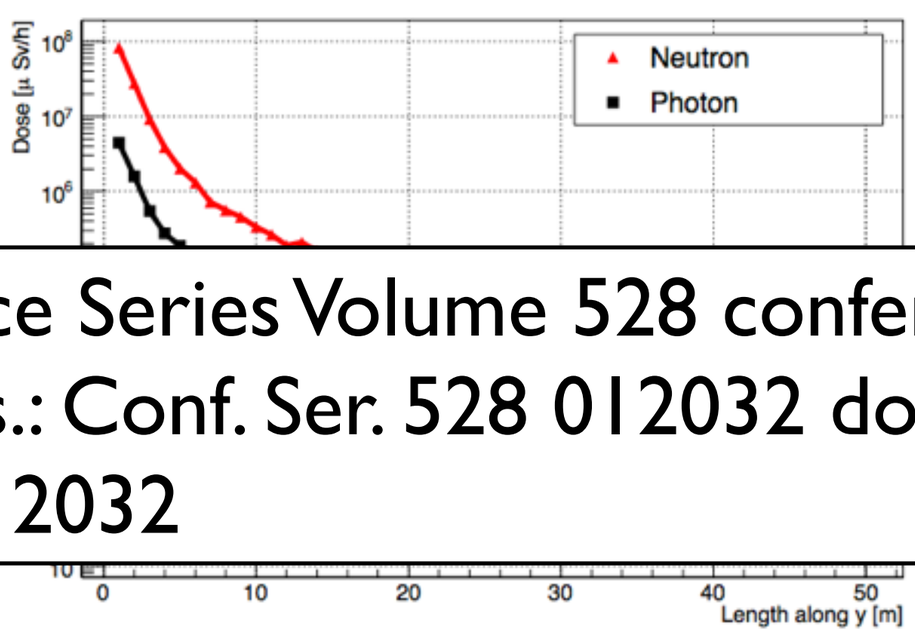

MCNPX

SSR SSW

McStas

# Use: Check the Scatter_logger.comp in the McStas distribution




Journal of Physics: Conference Series Volume 528 conference 1
E B Klinkby et al 2014 J. Phys.: Conf. Ser. 528 012032 doi: 10.1088/1742-6596/528/1/012032

# Future: Geant4, PHITS?

Collaboration
Nutech
Fysik

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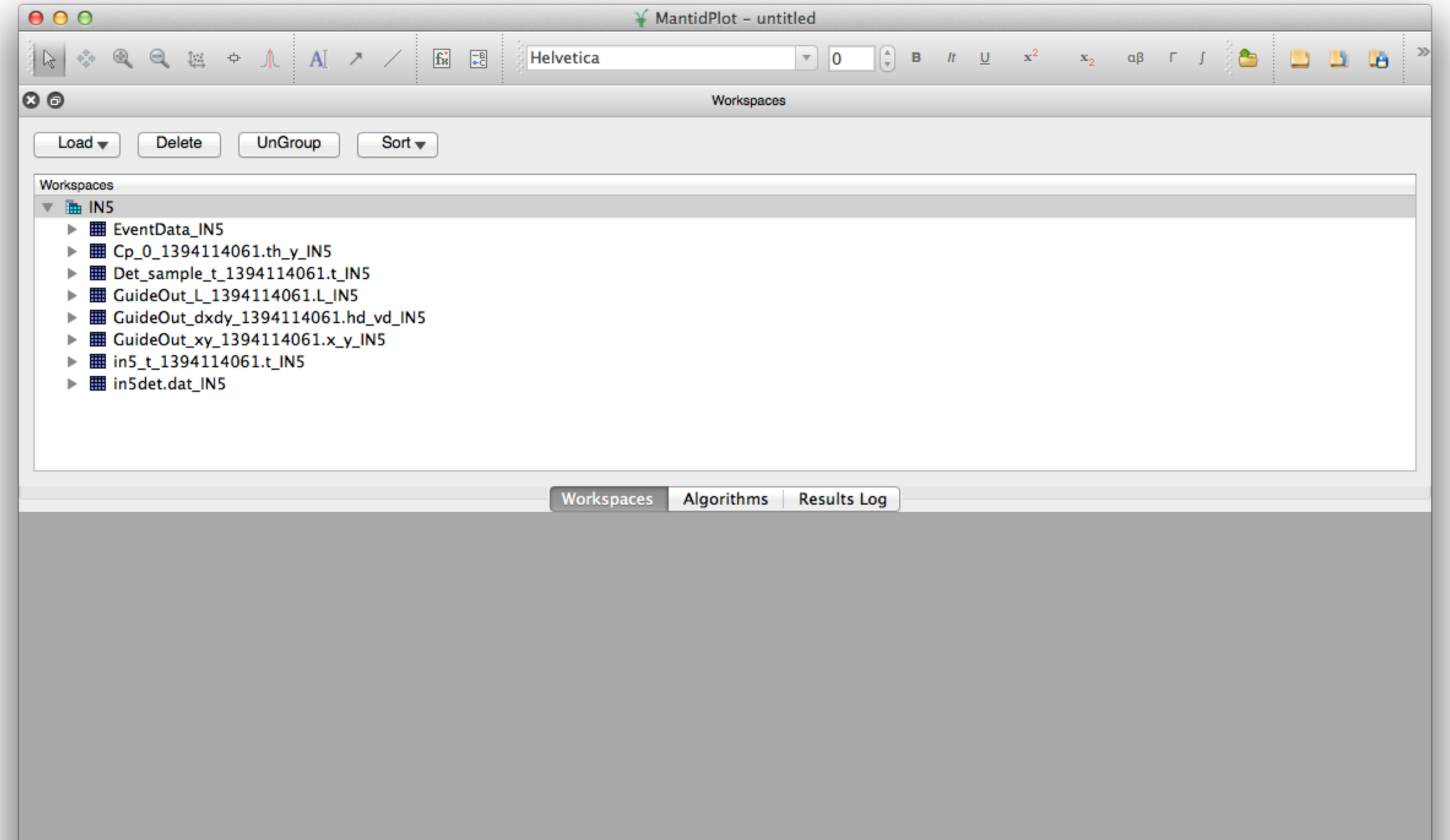
# McStas-Mantid event processing facilitated by:

Special labels in component list
Special Monitor_nD paramers
IDF autogenerated by “mcdisplay” run
NeXus output and LoadMcStas Mantid algorithm



# McStas-Mantid event processing facilitated by:

Special labels in component list
Special Monitor_nD paramers
IDF autogenerated by “mcdisplay” run
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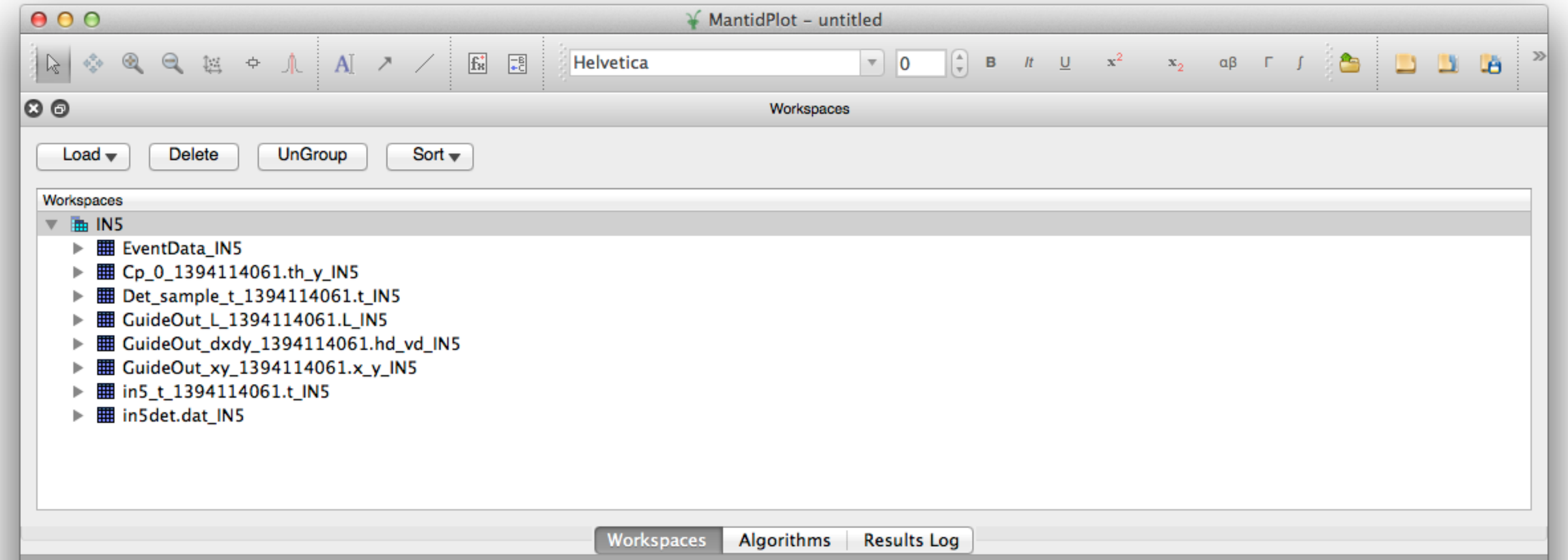
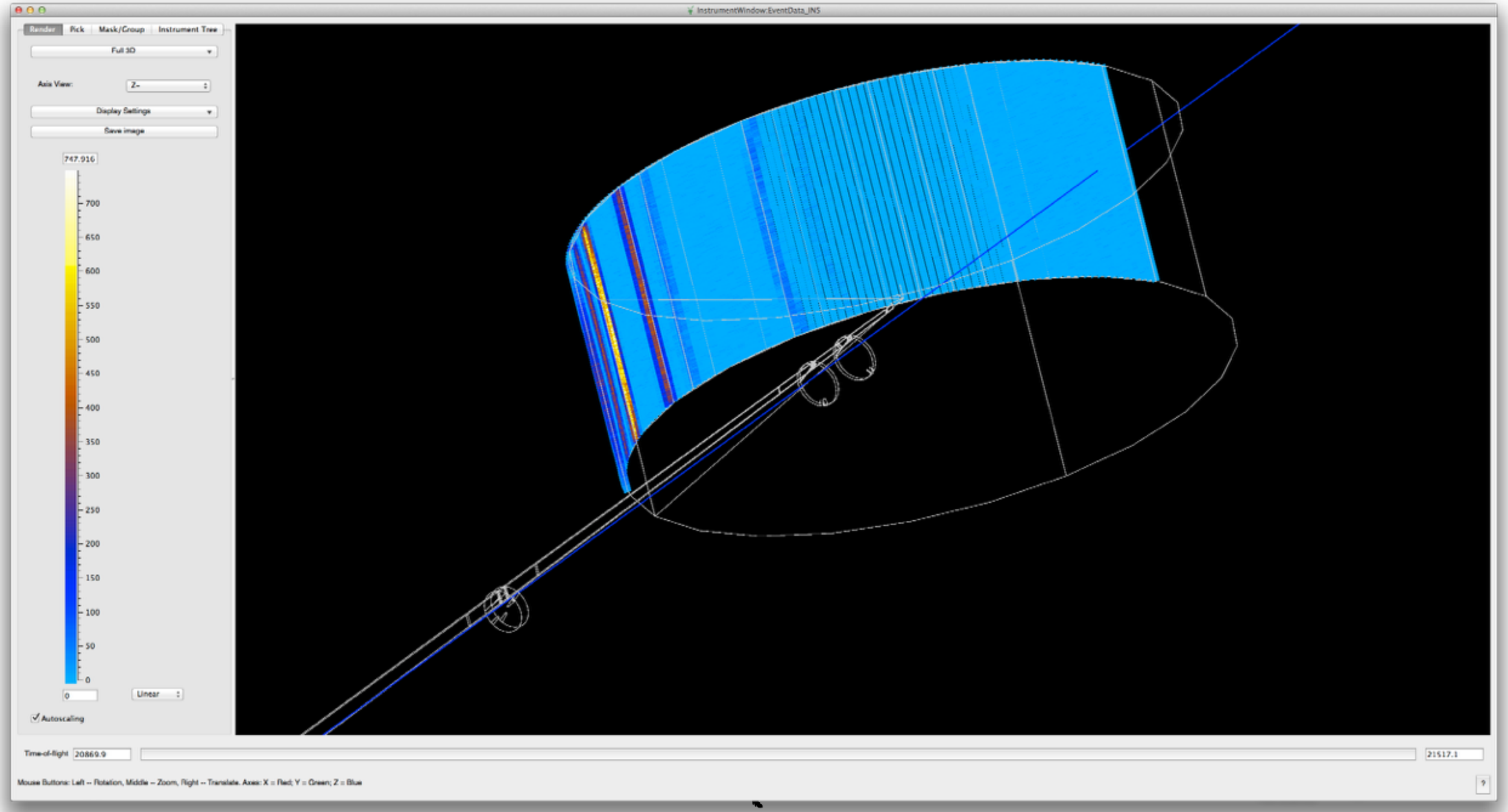



Use: Check out templateSANS_Mantid from the McStas distribution - fully functional reduction

# Events shown on the full instrument

- The event data from McStas should look something like this in “full 3D” - you may have to move/zoom a bit about



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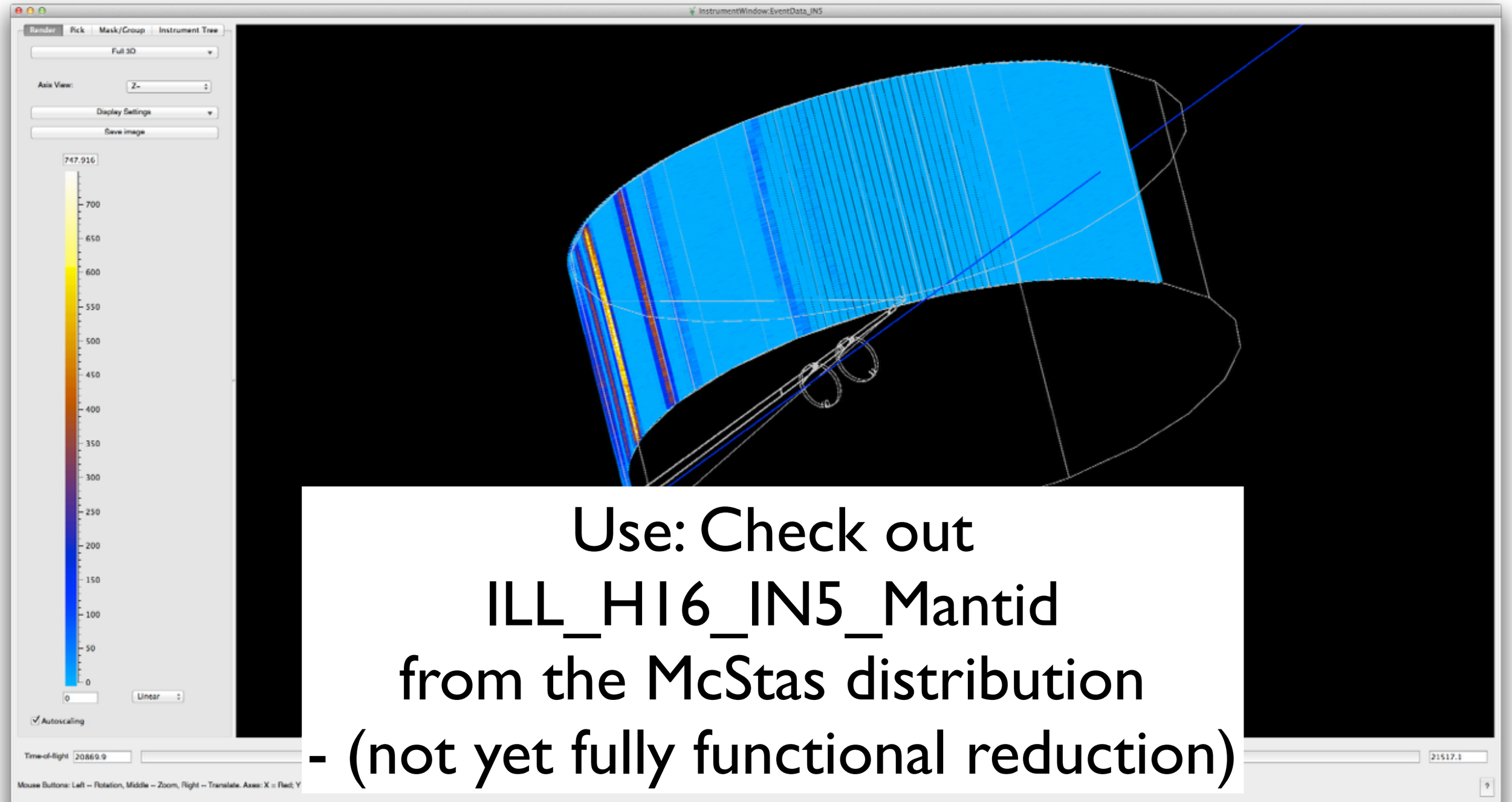
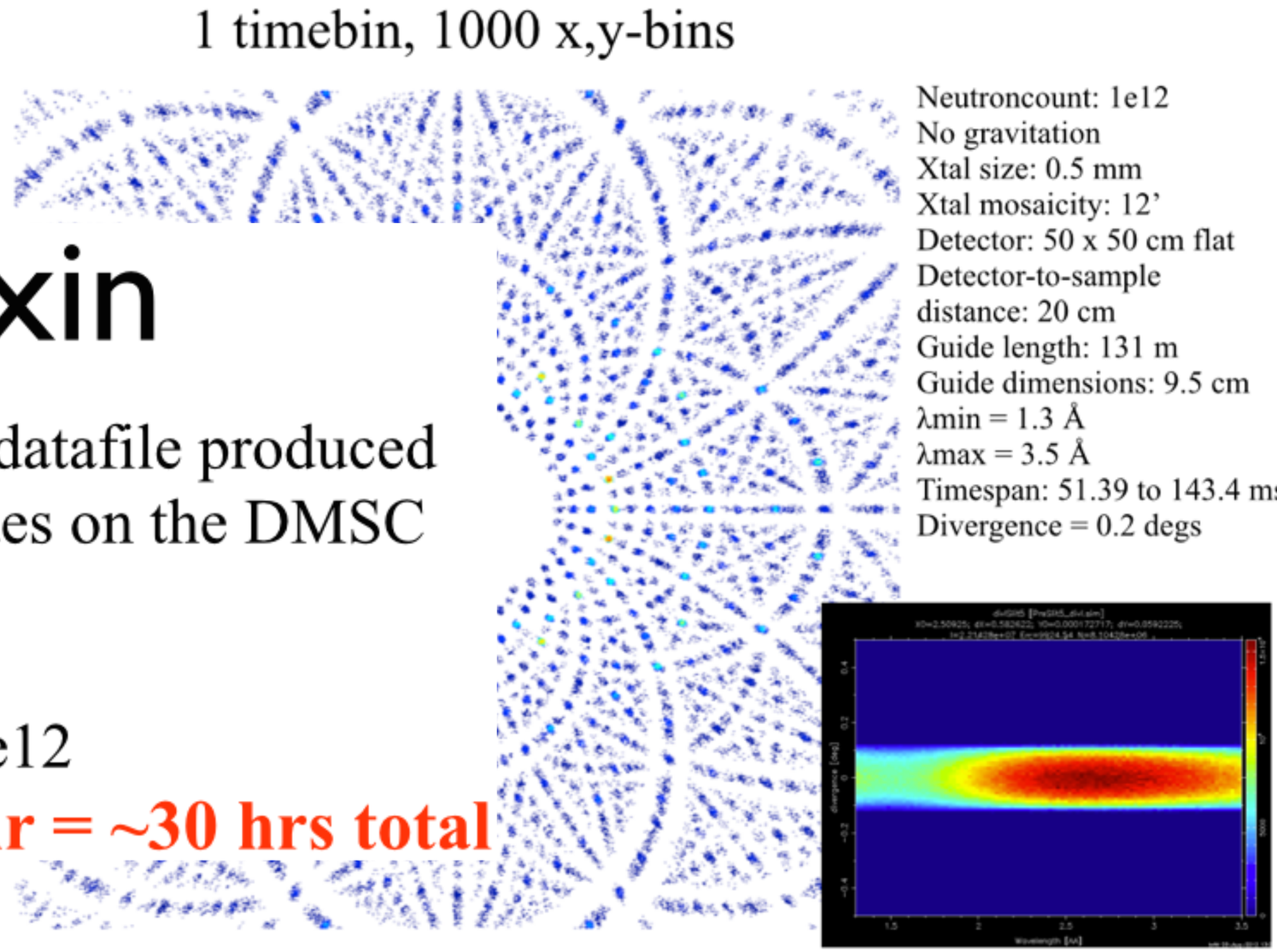


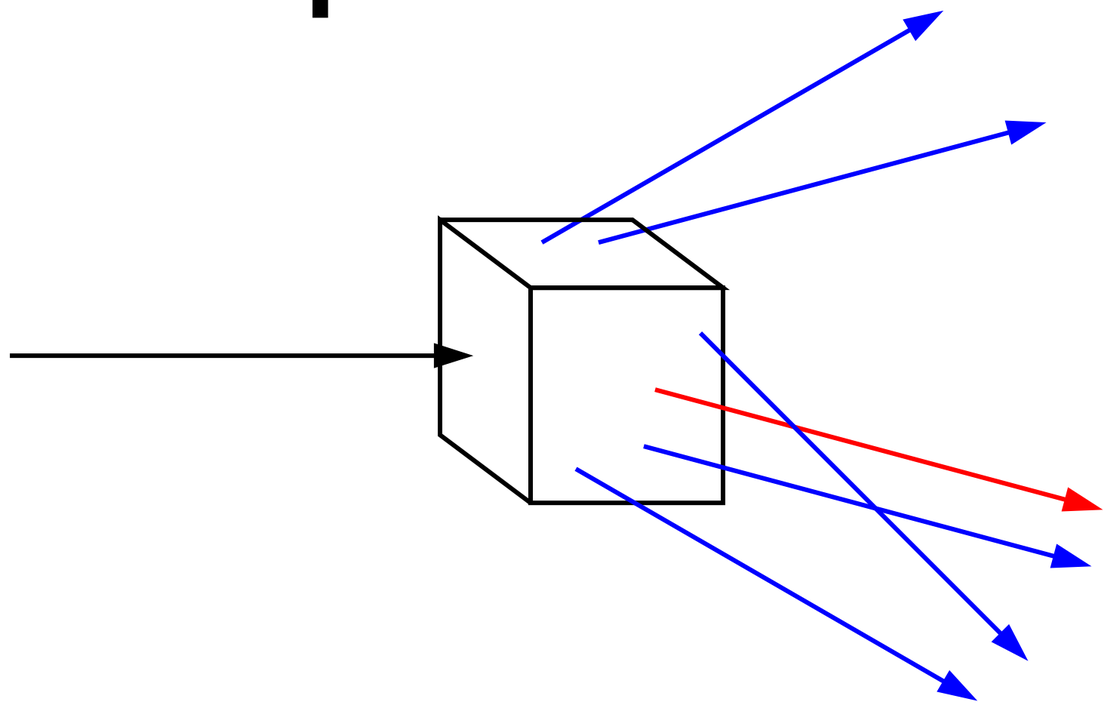
# Problem: McStas Single_crystal.comp "slow" for large unit cell diffraction studies

- Example: Rubredoxin




- Reflection list ~ 124 K reflections (still "small" in the PX world!!)

# Algorithm improvement: **Use incoming neutrons more efficiently - scatter each one on all possible reflections**



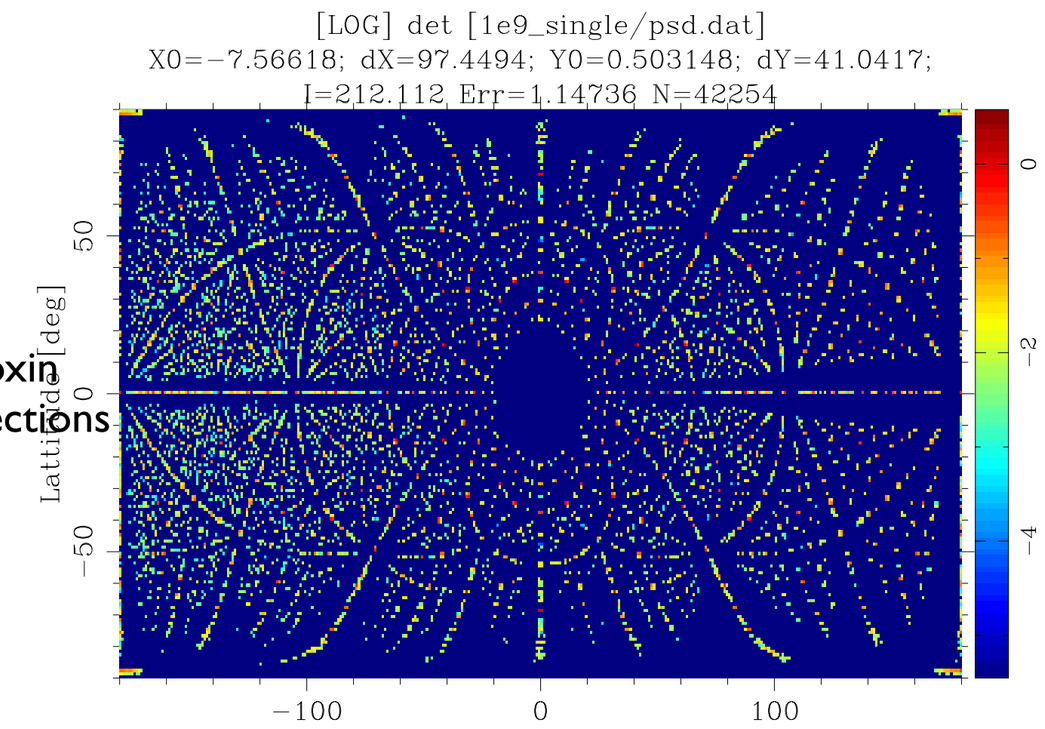
- **Red**: Original algorithm, one incoming neutron used only once
- **Blue**: Improved algorithm, each incoming neutron scattered (via SPLIT keyword) all possible times
- Component makes **estimate on average number of "active"** diffraction **spots** - in the case Rubredoxin this is around **50**!

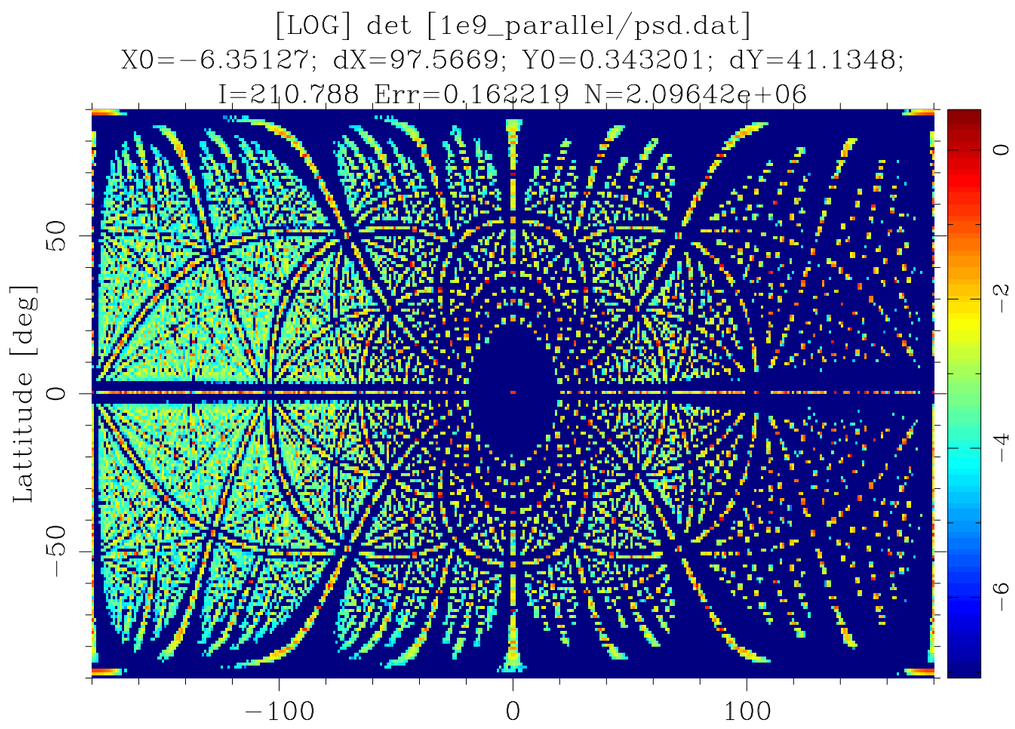
# Sim data speak for themselves - 1e9 rays

## Old comp

## New comp

Rubedoxin
124K reflections




~ Factor **50**
more efficient

Predeuterated
pyrophosphatase
1.7M reflections



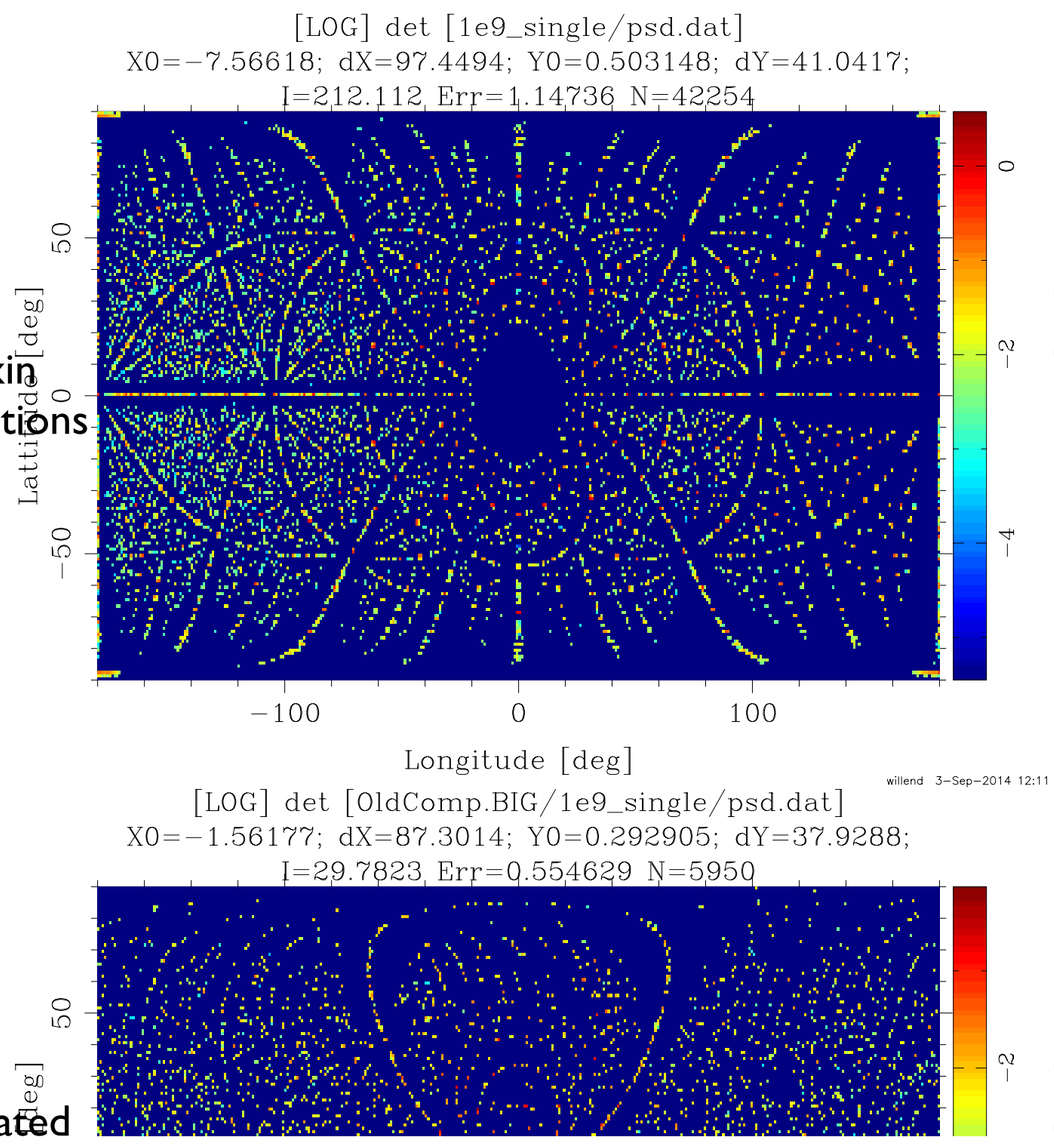




~ Factor **500**
more efficient

# Sim data speak for themselves - 1e9 rays

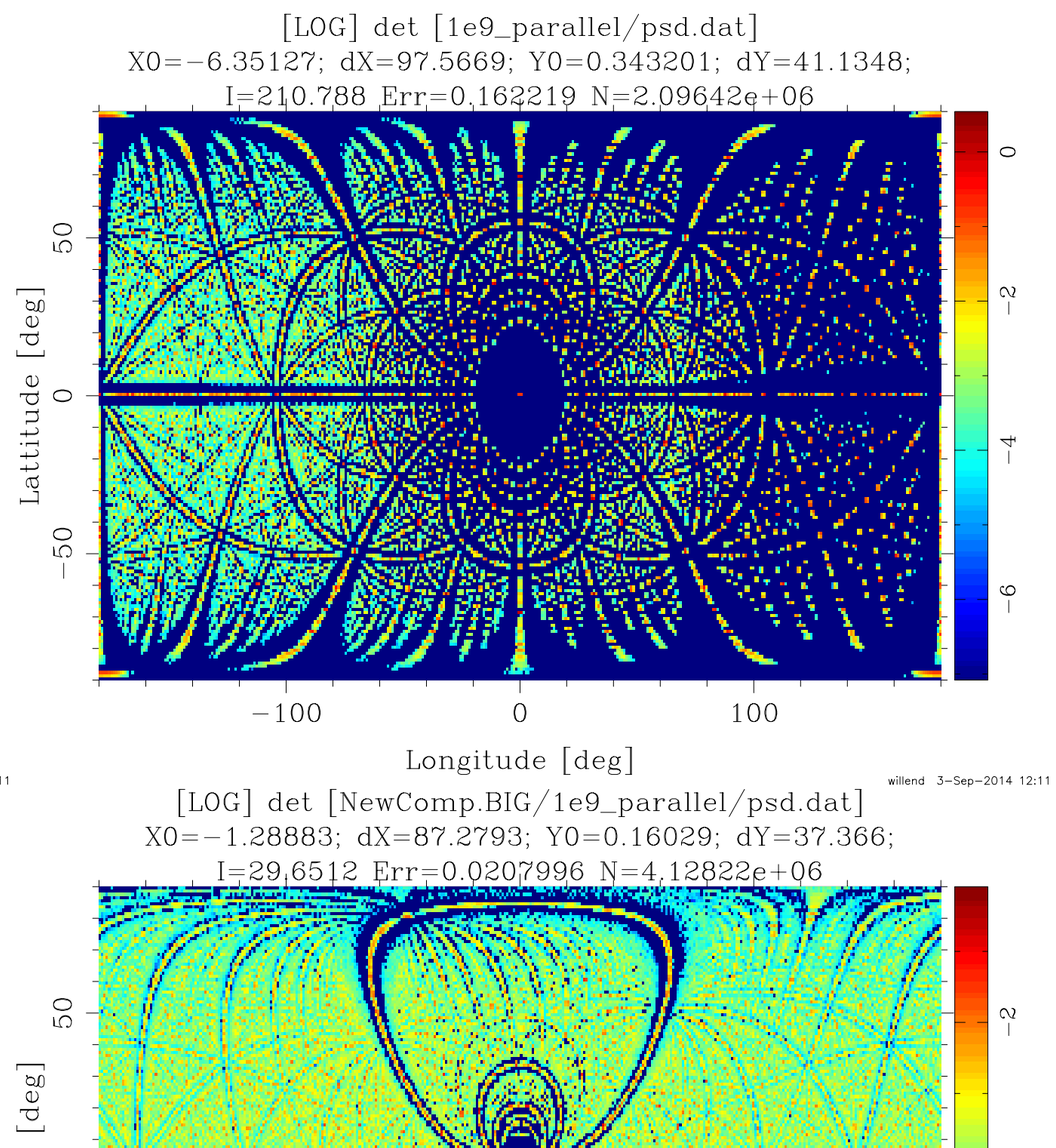
## Old comp




Rubedoxin
124K reflections

Predeuterated

## New comp




~ Factor **50** more efficient

~ Factor **500** more efficient

Use: Check out template_NMX from the McStas distribution

Similar optimisation of the PowderN component

# People

- The success of the project is also about the people:
  - Present McStas team members

- K Lefmann

E Farhi

P Willendrup

E Knudsen

U Filges

T R Nielsen

  - Past McStas team members

- K Nielsen

PO Åstrand

K Lieutenant

P Christiansen

J Brinch